Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 6.60

Global applicability domain: Inside

Local applicability domain index: 9.21e-01

Confidence level: 7.03e-01

Nearest Neighbors from the Training Set

Image not found
Pentachlorobenzene
Measured: 6.49
Predicted: 6.59

Image not found
Acenaphthene
Measured: 6.31
Predicted: 6.67

Image not found
1,2-Dichloronaphthalene
Measured: 6.89
Predicted: 6.90

Image not found
Biphenyl
Measured: 6.15
Predicted: 5.83

Image not found
trans-Stilbene
Measured: 7.48
Predicted: 6.90